

Intrinsic surface depression of the order parameter under mixed $(s + id)$ -wave pair symmetry and its effect on the critical current of high-Tc SIS Josephson junctions

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Abstract

An intrinsic gap depression at the Superconductor-Insulator interface due to the very short value of the coherence length in High-Tc Superconductors [HTSs] is considered, in the framework of a mixed $(s+id)$ -wave pair symmetry for the order parameter ranging from pure s to pure d -wave. This gap depression acts as the main physical agent causing the relevant reduction of $I_c(T)R_n(T)$ values with respect to BCS expectations in HTS SIS Josephson junctions. Good agreement with various experimental data is obtained with both pure s -wave and pure d -wave symmetries of the order parameter, but with amounts of gap depression depending on the pair symmetry adopted. Regardless of the pair symmetry considered, these results prove the importance of the surface order-parameter depression in the correct interpretation of the $I_c(T)R_n(T)$ data in HTS SIS junctions. In a case of planar YBCO-based junction the use of the de Gennes condition allowed us to tentatively obtain an upper limit for the amount of d -wave present in the gap of YBCO. PACS numbers: 74.50.+r; 74.70.Vy

KEY WORDS: High-Tc superconductors; Order parameter; Josephson junctions; Josephson critical current; Pair symmetry.

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As a consequence of the very short coherence length ξ of high-Tc superconductors [HTSs], an intrinsic depression of the order-parameter at Superconductor-Insulator [S-I] interfaces arises [1], which can represent one of the main reason for the reduced $I_c(T)R_n(T)$ values in HTS SIS [2,3] and SIS' Josephson junctions [4].

Also pair symmetry is expected to contribute to such experimental results, and, in the present paper, a model is developed by us which takes into consideration pure s -wave, pure d -wave and mixed $(s + id)$ -wave pair symmetry together with a suitable gap depression, extending and generalizing our previous model developed for $T > 0$ only in the pure s -wave case [3,4].

By making use of the space-dependent expression of the gap $\Delta(x, T) = \Delta(T) \tanh \left[(x + x_0) / (\sqrt{2}\xi(T)) \right] \cdot \theta(x - w)$ which may be derived from Ginzburg-Landau equations, $I_c(T)R_n(T)$ values in SIS and SIS' Josephson junctions [JJs] may be evaluated. Here $2w$ is the thickness of the insulating layer and x_0 accounts for the spatial slope of $\Delta(x, T)$ near interfaces [4]. As in Ref. [5] we assume that the d -wave component of the order parameter Δ_d has the same spatial behaviour as the s -wave component Δ_s and, moreover, we neglect the fourth-order terms in the Ginzburg-Landau equations for the $(s + id)$ -wave pair symmetry. We imagine to "section" the gap $\Delta(x, T)$ into independent channels $\delta\Delta_i$ [3,4], each of them giving rise to a parallel contribution $\delta I_{c_i}(T)$ and $\delta G_{n_i}(T)$ to the total critical current and normal conductance, respectively. The physical situation just described is depicted in Fig. 1 where our model for a HTS SIS Josephson junction is shown. By summing and averaging over all the parallel contributions, that in general differ since each "slice" corresponds to a different thickness of the barrier (see Fig. 1), we obtain:

$$I_c(T) \simeq \frac{1}{\Delta(T)} \sum_i [I_{c_i}(T) \cdot \delta\Delta_i(x, T)]$$

$$G_n(T) \simeq \frac{1}{\Delta(T)} \sum_i [G_{n_i}(T) \cdot \delta\Delta_i(x, T)]$$

In the continuous limit these expressions become:

$$I_c(T) = \frac{1}{\Delta(T)} \int_0^\infty I_c(x, T) \frac{\partial \Delta(x, T)}{\partial x} dx$$

$$G_n(T) = \frac{1}{\Delta(T)} \int_0^\infty G_n(x, T) \frac{\partial \Delta(x, T)}{\partial x} dx$$

and

$$[G_n(x, T)]^{-1} = R_n(x, T) = R_0(T) \cdot 10^{2(\frac{x}{w} - 1)}$$

where R_0 is a parameter representing the resistance of the channel at $x = w$, which gets eliminated after performing the integral for $G_n(T)$, and where the space dependence of $R_n(x, T)$ has been heuristically derived under global conditions of consistency [3]. The expression for the spatial dependence of $I_c(T)$ in mixed $(s+id)$ -wave symmetry is derived by introducing the spatial dependencies of Δ_s and Δ_d in the results of Ref. [6] :

$$I_c(x, T) = \frac{T}{e\pi \cdot R_n(x, T)} \sum_{l=1}^{\infty} \frac{4\Delta_s^2(x, T) + \Delta_d^2(x, T)}{\omega_l^2 + \Delta_s^2(x, T) + \Delta_d^2(x, T)} \left[K \left(\frac{\Delta_d(x, T)}{\sqrt{\omega_l^2 + \Delta_s^2(x, T) + \Delta_d^2(x, T)}} \right) \right]^2 \quad (1)$$

where $\omega_l = (2l - 1)\pi k_B T$ is the Matsubara frequency and K is the complete elliptic integral of the first kind.

After performing rather cumbersome calculations, the general expression for the temperature dependent critical voltage $I_c(T)R_n(T)$ in the case of SIS JJs, in mixed $(s+id)$ -wave symmetry and in presence of surface depression of the order parameter is given by:

$$[I_c(T)R_n(T)]_{SIS}^{(s+id)+dep.gap} = \frac{4k_B T}{e\pi} \cdot A(T) \cdot \sum_{l=1}^{\infty} \left[B(l, T) \cdot K_\gamma^2(l, T) + \int_{\gamma(T)}^1 C(l, T, z) \cdot K_z^2(l, T, z) \cdot dz \right] \quad (2)$$

where

$$A(T) = \frac{1}{\gamma(T) \left(\frac{1-\gamma(T)}{1+\gamma(T)} \right)^{\vartheta(T)} + \int_{\gamma(T)}^1 dz \left(\frac{1-z(T)}{1+z(T)} \right)^{\vartheta(T)}}$$

$$B(l, T) = \frac{\gamma^3(T) \left(\frac{1-\gamma(T)}{1+\gamma(T)} \right)^{\vartheta(T)} [4\Delta_s^2(T) + \Delta_d^2(T)]}{\omega_l^2 + \gamma^2(T) (\Delta_s^2(T) + \Delta_d^2(T))}$$

$$C(l, T, z) = \frac{z^2(T) \left(\frac{1-z(T)}{1+z(T)}\right)^{\vartheta(T)} [4\Delta_s^2(T) + \Delta_d^2(T)]}{\omega_l^2 + z^2(T) (\Delta_s^2(T) + \Delta_d^2(T))}$$

$$K_\gamma(l, T) = K \left(\frac{\Delta_d(T) \gamma(T)}{\sqrt{\omega_l^2 + \gamma^2(T) (\Delta_s^2(T) + \Delta_d^2(T))}} \right)$$

$$K_z(l, T, z) = K \left(\frac{\Delta_d(T) z(T)}{\sqrt{\omega_l^2 + z^2(T) (\Delta_s^2(T) + \Delta_d^2(T))}} \right)$$

$$\text{and } z(x, T) = \tanh\left(\frac{x+x_0}{\xi(T)\sqrt{2}}\right), \gamma(T) = \tanh\left(\frac{w+x_0}{\xi(T)\sqrt{2}}\right), \vartheta(T) = \xi(T)\left(\frac{\ln(100)}{w\sqrt{2}}\right).$$

In the previous expressions we considered $\Delta_s(T) = (1 - \varepsilon) \cdot \Delta_{ex}(T)$ and $\Delta_d(T) = \varepsilon \Delta_{ex}(T)$ where ε is the fraction of d -wave present in the order parameter, Δ_{ex} is the experimental value of the gap determined, for example, in tunneling experiments [7,8] and where we have used for the temperature dependence of $\Delta(T)$ and $\xi(T)$ the standard BCS expressions. In the special case of pure s -wave pair symmetry Eq. (2) reduces to [3]:

$$[I_c(T)R_n(T)]_{SIS}^{pure\ s+dep.\ gap} = \frac{\pi\Delta_s(T)}{e} \frac{\left[\frac{\gamma^2}{2} \left(\frac{1-\gamma}{1+\gamma}\right)^\vartheta \tanh\left(\frac{\gamma\Delta_s(T)}{2k_B T}\right) + \int_\gamma^1 z \left(\frac{1-z}{1+z}\right)^\vartheta \tanh\left(\frac{z\Delta_s(T)}{2k_B T}\right) dz \right]}{\gamma \left(\frac{1-\gamma}{1+\gamma}\right)^\vartheta + \int_\gamma^1 \left(\frac{1-z}{1+z}\right)^\vartheta dz}$$

which tends to the Ambegaokar-Baratoff [AB] model [9] in the limits valid for a low-T_c superconductor (LTS) (i.e. $x_0 \rightarrow +\infty, \xi(0) \rightarrow +\infty, x_0/\xi(0) \rightarrow +\infty$):

$$\lim_{HTS \rightarrow LTS} [I_c(T)R_n(T)]_{SIS}^{pure\ s+dep.\ gap} = \frac{\pi\Delta_s(T)}{2e} \tanh\left(\frac{\Delta_s(T)}{2k_B T}\right).$$

When gap depression at S-I interfaces is neglected, the result obtained by Xu et al. [6] in the general mixed $(s+id)$ -wave case is reproduced:

$$[I_c(T)R_n(T)]_{SIS}^{s+id} = \frac{T}{e\pi} \cdot \sum_{l=1}^{\infty} \frac{4\Delta_s^2(T) + \Delta_d^2(T)}{\omega_l^2 + \Delta_s^2(T) + \Delta_d^2(T)} \cdot \left[K \left(\frac{\Delta_d(T)}{\sqrt{\omega_l^2 + \Delta_s^2(T) + \Delta_d^2(T)}} \right) \right]^2.$$

On the other hand, in the case of pure d -wave pair symmetry and in presence of a depression of the order parameter all the components of Eq. (2) reduce to the analogous expressions for $\Delta_s(T) = 0$ (i.e. $\varepsilon = 1$):

$$[I_c(T)R_n(T)]_{SIS}^{pure\ d+dep.\ gap} = \lim_{\Delta_s \rightarrow 0} [I_c(T)R_n(T)]_{SIS}^{(s+id)+dep.\ gap}.$$

We remark that the free parameters of the model expressed by Eq. (2) in the most general case are three: w , x_0 and ε . When the thickness of the insulating barrier is known (for example in planar SIS JJs) the number of free parameters reduces to two. It becomes only one if, in a planar SIS junction, the amount of d -wave is also fixed as in the pure s -wave case ($\varepsilon = 0$) or in the pure d -wave one ($\varepsilon = 1$).

A reasonable estimation of the minimum (intrinsic) amount of gap depression present at S-I interfaces may be obtained by calculating the x_0 value - from now on called x_0^{dG} - that derives from the de Gennes condition at the S-I interface [10]:

$$\left[\frac{d\Delta(x)}{dx} \right]_{x=w} = \left[\frac{1}{b} \Delta(x) \right]_{x=w}$$

where, in the hypothesis of Ginzburg-Landau behaviour for $\Delta(x)$, we have

$$\frac{1}{b} = \frac{\sqrt{2}}{\xi(0)} \frac{1}{\sinh\left(2\frac{w+x_0^{dG}}{\xi(0)\sqrt{2}}\right)}.$$

The previous expression, together with the approximate value $b \simeq \xi^2(0) / (a - w)$ determined by de Gennes, where a is the range of the x axis where $\Delta(x)$ varies appreciably [10], permits to calculate x_0^{dG} . When, due to a short $\xi(0)$, a large intrinsic gap depression at S-I interfaces is expected, $\frac{w+x_0^{dG}}{\xi(0)\sqrt{2}} < 0.4$ so that $b \simeq w + x_0^{dG}$. This condition is always satisfied in the HTS junctions we will describe thereafter. If we impose that $\Delta(a, T) / \Delta(\infty, T) = 0.99$, considering that $0.99 \simeq \tanh 2.6$, a value of a may be yielded so that an estimate for x_0^{dG} is obtained by means of $x_0^{dG} \simeq 0.6 \cdot \xi(0) - w$. In principle, the x_0 values determined by fitting the experimental data with our depressed-gap model have to be comprised between x_0^{dG} and $x_0 = -w$ that corresponds to a complete gap depression at the interface i.e. $\Delta(w) = 0$.

Agreement of such a model with experimental $I_c(T)R_n(T)$ data in HTS SIS JJs has been tested for the two cases of pure s -wave and pure d -wave pair symmetry. On the other hand, a fit of the experimental curves by the complete $(s+id)$ -wave model in absence of indications concerning the amplitude of the d -wave component of the gap would have been of very modest interest due to the numerical impossibility to separate the contributions of the gap depression x_0 and of the d -wave gap ε to the lowering of $I_c(T)R_n(T)$. As we will

see in the following examples, results are very good with both types of pair symmetry, but with a different amount of gap depression in each case.

Examples presented in this work include one of our recent $I_c(T)R_n(T)$ behaviours obtained from reproducible nonhysteretic I - V curves in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ ($T_c = 85$ K, $\Delta_{BSCCO}(0) = 23$ meV, $\xi_{BSCCO}(0) = 1.67$ nm) single-crystal high-quality Josephson break junctions (Fig.2). RSJ model [11] has been used to obtain $I_c(T)$ and $R_n(T)$ values as these latter were high enough to permit to treat the junctions as tunnel SIS ones [3,12]. Best-fit values for the amount of the gap depression are $(x_0)_s = -1.75$ nm and $(x_0)_d = 0.5$ nm, while the thickness of the barrier, fitted by using the pure s -wave expression and held constant also for the pure d -wave case, is $2w = 4.4$ nm. Figure 2 shows the results of the fit of experimental data by using the depressed-gap model compared to the standard BCS results (no gap depression) in s - and d -wave symmetry. As in all the figures from 2 to 5, open symbols are experimental $I_c(T)R_n(T)$ data, dash-dots and dots represent predictions obtained considering pure s -wave (AB model [9]) and pure d -wave pair symmetry *without* any gap depression, respectively, while the results of our model applied to the pure s -wave and the pure d -wave cases are reported with a dashed and continuous line, respectively. In all the presented cases the superconducting gap $\Delta(0)$ has been determined from tunneling experiments or from literature while the coherence length $\xi(0)$ was taken from literature.

The depressed-gap model has been tentatively used also in $\text{Bi}_2\text{Sr}_2\text{CuO}_{6+x}$ (Bi-2201) single-crystal break-junctions [13] where $T_c = 9.6$ K, $\Delta_{BSCO}(0) = 3$ meV and $\xi_{BSCO}(0) = 4$ nm. The results of the fits in these nonhysteretic Bi-2201 break-junctions are shown in Fig. 3 and the fitted values of the gap depression are equal to $(x_0)_s = -4.0$ nm, $(x_0)_d = 0.5$ nm. The barrier thickness, as usual determined by the s -wave depressed-gap fit, is $2w = 9.8$ nm.

Fig. 4 reports data taken from a SIS YBCO-based bicrystal grain-boundary junction fabricated on a SrTiO_3 (STO) substrate [14] and fitted by our model with a barrier thickness, determined as in the previous cases, $2w = 2.0$ nm. Here the amounts of gap depression are $(x_0)_s = -0.6$ nm and $(x_0)_d = 1.0$ nm, while $T_c = 85$ K, $\Delta_{YBCO}(0) = 16$ meV and $\xi_{YBCO}(0) = 2.8$ nm.

Fig. 5 reports the case of a YBCO/STO/YBCO multilevel edge JJ [15,4] with *ex situ* oxygen plasma treatment, which is well fitted by our model (both *s*- and *d*-wave symmetry) with only one adjustable parameter, being $2w = 7.2$ nm already known independently from the fabrication process. The fitted values of the parameter x_0 are $(x_0)_s = -3.3$ nm and $(x_0)_d = -0.4$ nm. The physical values characteristic of the superconducting state used in the fit are: $T_c = 85$ K, $\Delta_{YBCO}(0) = 16$ meV and $\xi_{YBCO}(0) = 2.8$ nm. It is clear from Figs. 2 to 5 that both the *s*-wave and the *d*-wave depressed-gap curves fit properly the magnitude and, in most of the cases, also the shape of the various experimental $I_c(T)R_n(T)$ data, but with different amounts of gap depression: pure *d*-wave fit requires a smaller amount of surface gap depression (i.e. a larger value of x_0) than pure *s*-wave one.

In the latter junction, taking advantage of the *a priori* knowledge of the exact value of w , the behaviour of the amount of gap depression (accounted for by x_0) vs. ε (percentage of *d* wave) has been obtained by using the general mixed $(s+id)$ -wave model of Eq. (2) and reported in Fig. 6. Since in that case $x_0^{dG} \simeq -1.9$ nm, from the graph of Fig. 6 a pure *d*-wave would be excluded, and an upper limit of the order of 40% for the percentage of *d*-wave pair symmetry in YBCO is draftily given. Anyway we must remark that the results are very sensitive to the gap value and, therefore, different values for Δ_{YBCO} (such as 20 meV rather than the 16 meV we used following the authors of Ref. [15]) would yield for x_0 values compatible also with a pure *d*-wave pair symmetry. The x_0^{dG} values, calculated by means of the above mentioned approximate expression for the junctions of Fig. 2, 3 and 4, are always comprised between $(x_0)_s$ and $(x_0)_d$. Even considering the mentioned sensitivity of the results to the value of the gap and to the value of w , this fact seems to indirectly question the presence of pure *d*-wave symmetry in the HTS materials of these junctions.

With this extension of our model, any comparison with the experimental results of SIS' JJs [16,17] (where S' is a low- T_c superconductor) is no longer meaningful due to the orthogonality between wave functions with symmetries *s* and *d*. Actually, the mere detection of a Josephson current in SIS' JJs rules out the existence of pure *d*-wave pair symmetry. Only depressed-gap pure *s*-wave symmetry [4] or mixed $(s+id)$ -wave pair symmetry plus order-

parameter depression can be acceptable in SIS' JJs. In the latter case, if the ratio Δ_d/Δ_s is not fixed (i.e., if it's a free parameter of the model), its effect in reducing $I_c(T)R_n(T)$ values becomes not distinguishable and not separable from the effect eventually operated by a S-I gap depression. On the other hand, considering the ratio Δ_d/Δ_s as a free, adjustable parameter leads to an unphysical sample-dependence of the pair symmetry which does not appear acceptable.

A first conclusion is therefore the full confirmation of the important role played by a surface gap depression in reducing the "quality factor" $I_c(T)R_n(T)$ below its theoretical BCS value (regardless of the type of gap symmetry considered) in HTS SIS Josephson junctions. As it is shown in Figs. 2 to 5 and in the framework of our model there is no possibility to fit the shape and, especially, the magnitude of experimental data by using pure s -wave, pure d -wave or mixed $(s+id)$ -wave models without any gap depression. Moreover, we remark that fitting of reduced $I_c(T)/I_c(0)$ values rather than $I_c(T)$ ones is not meaningful - even if very often present in literature - since the main discrepancy of experimental results from theoretical predictions is in the *magnitude* rather than in the *shape* of the curves.

As we have shown in the previous examples, the value of x_0 accounting for the depression of the order parameter depends on the type of pair symmetry adopted and, therefore, we can also conclude that - when applied to several experimental results - this model might yield a contribution to the pair symmetry debate only provided the amount of gap depression at S-I interface in each case examined is given independently from other measurements or physical considerations, and is not a free, adjustable parameter as we have treated it in our present calculations.

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FIGURES

FIG. 1. Surface-depressed order parameter $\Delta(x, T)$ as function of x and a "slice" $\delta\Delta_i$ into which we imagine to section the gap, in order to compute $I_c(T)R_n(T)$ in SIS JJs.

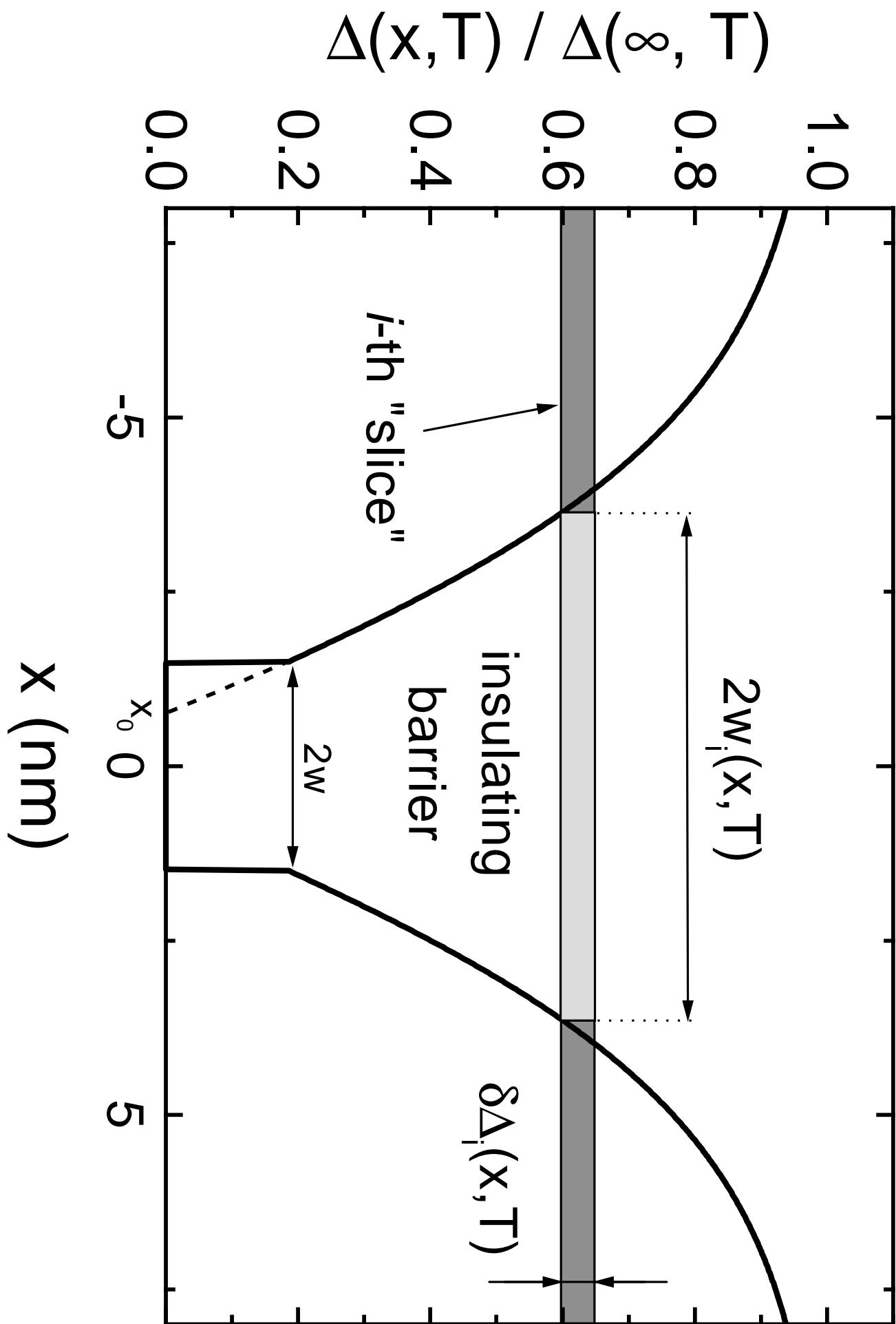
FIG. 2. Comparison of the experimental $I_c(T)R_n(T)$ obtained from a $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ single-crystal Josephson break junction with the curves yielded by various theoretical models (see text): open symbols are experimental data; dash-dots and dots represent predictions obtained considering pure s -wave and pure d -wave pair symmetry without gap depression, respectively, while the results of our model both in the pure s -wave and in the pure d -wave cases are reported with a dashed and continuous line, respectively.

FIG. 3. Comparison of the $I_c(T)R_n(T)$ behaviour obtained from a $\text{Bi}_2\text{Sr}_2\text{CuO}_{6+x}$ single-crystal break-junction with the results of various models as shown in Fig. 2.

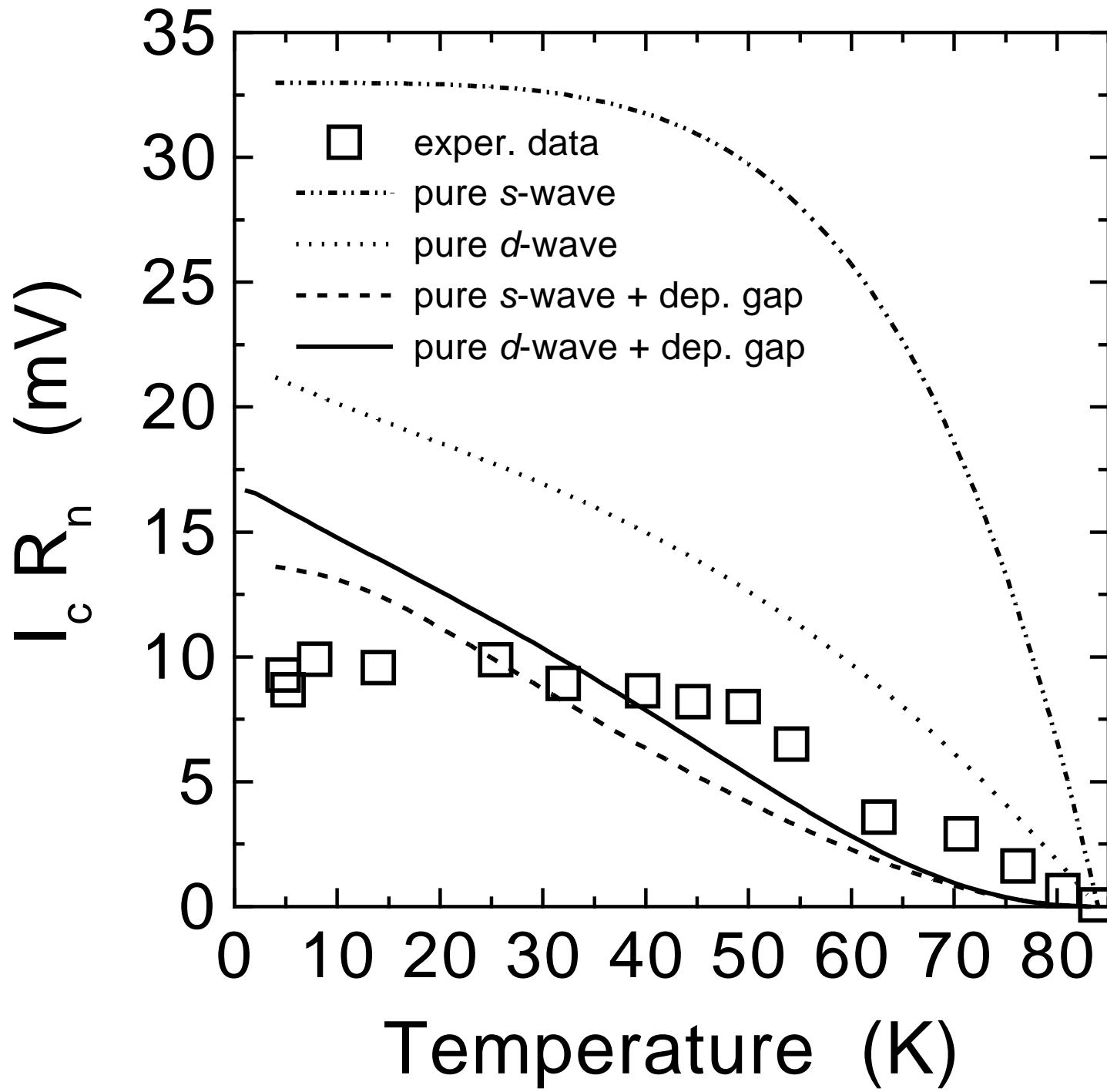
FIG. 4. The same as in Figs. 2 and 3 but with the $I_c(T)R_n(T)$ data taken from a YBCO-based bicrystal grain-boundary junction fabricated on SrTiO_3 substrates (from Ref. [14]).

FIG. 5. The same as in Figs. 2 - 4 but with the experimental $I_c(T)R_n(T)$ data taken from a SIS YBCO/STO/YBCO multilevel edge JJ (from Ref. [15]) and fitted by our model with only one adjustable parameter.

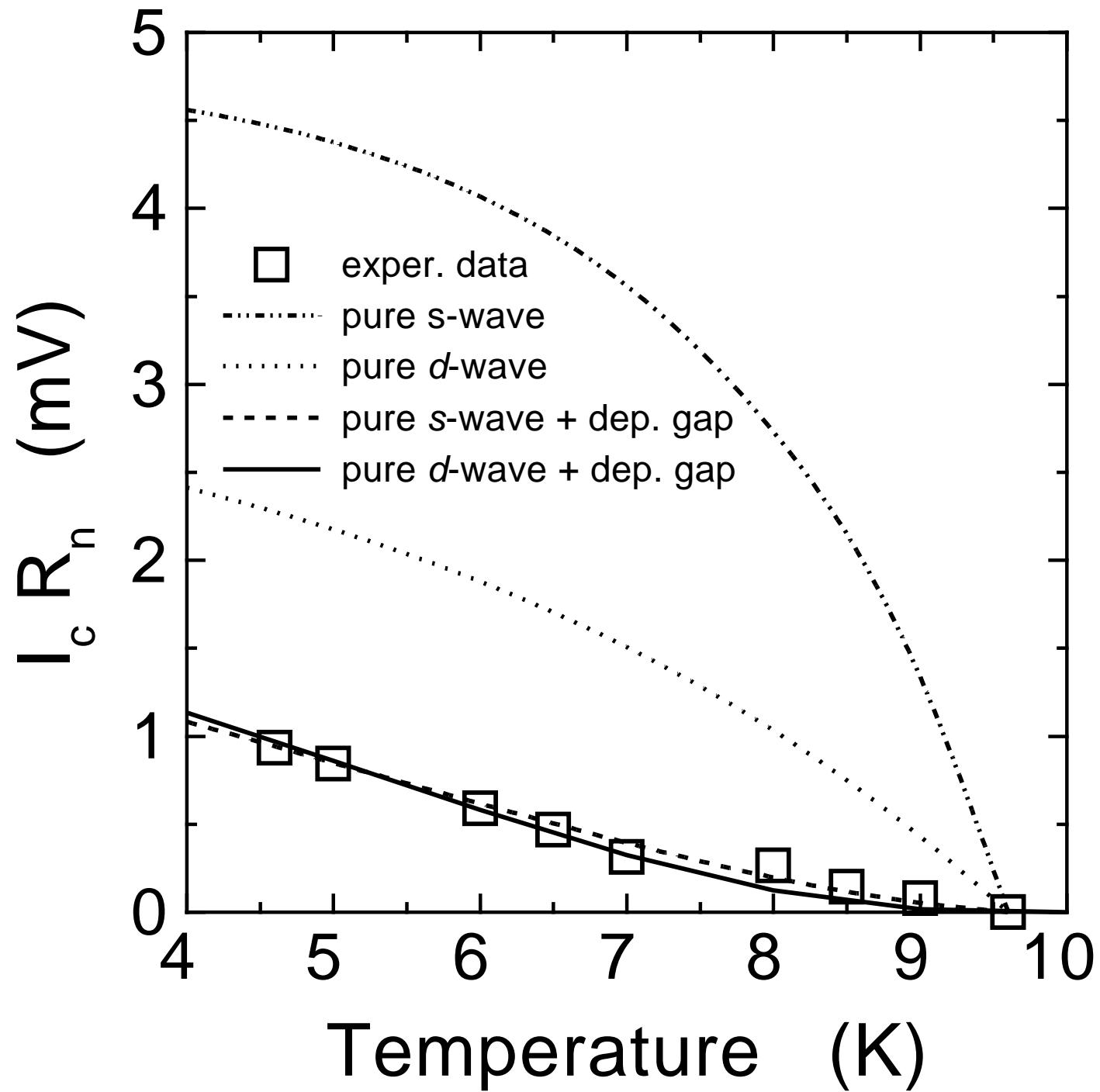
FIG. 6. Behaviour of the amount of gap depression (accounted for by x_0) vs. percentage of d wave (in the general mixed $(s + id)$ -wave model), estimated taking advantage of the *a priori* knowledge of the barrier thickness $2w$ in the case of Fig. 5.



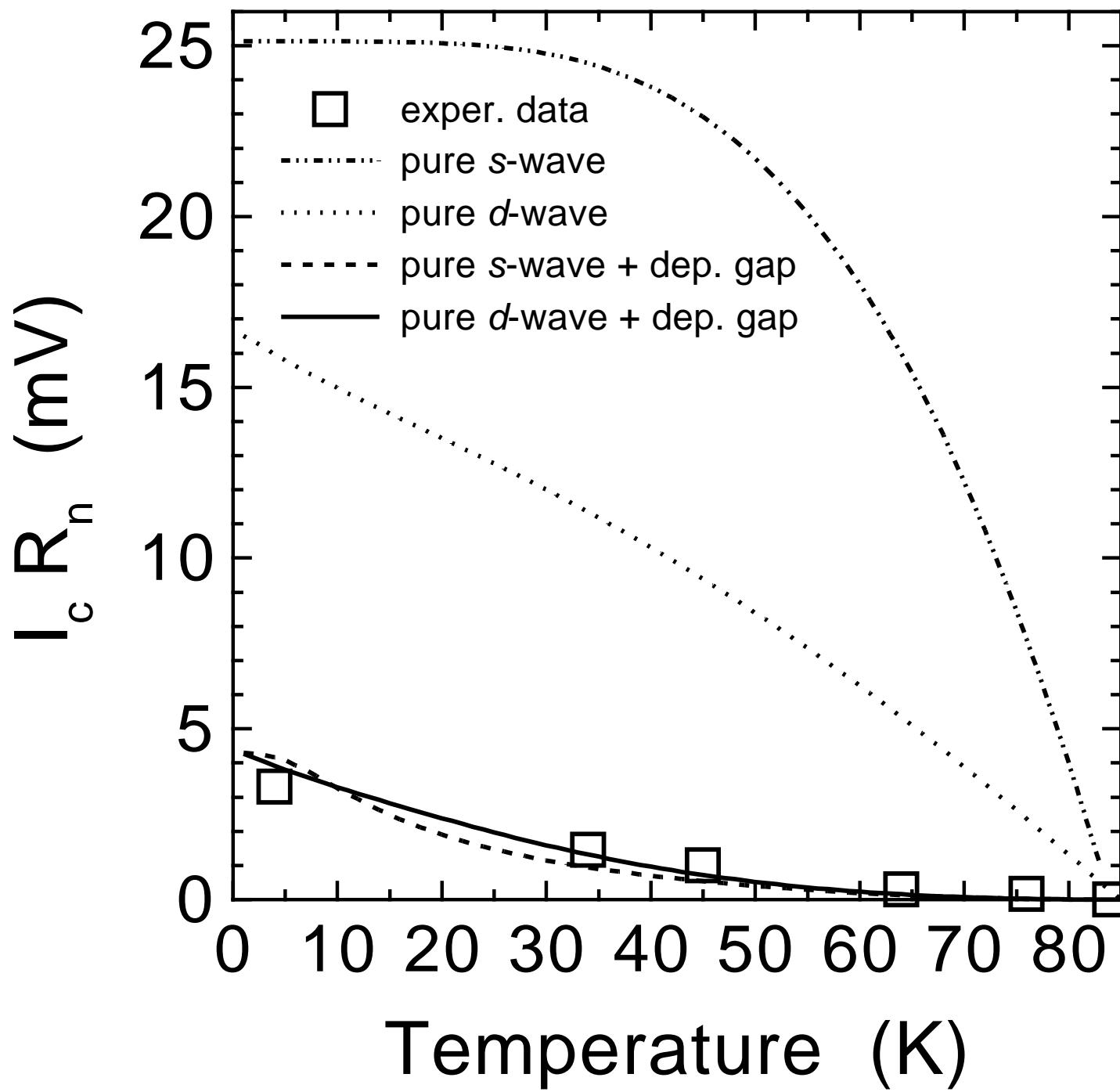
G.A. Ummarino et al., "Intrinsic surface depression of the ...", Fig. 1



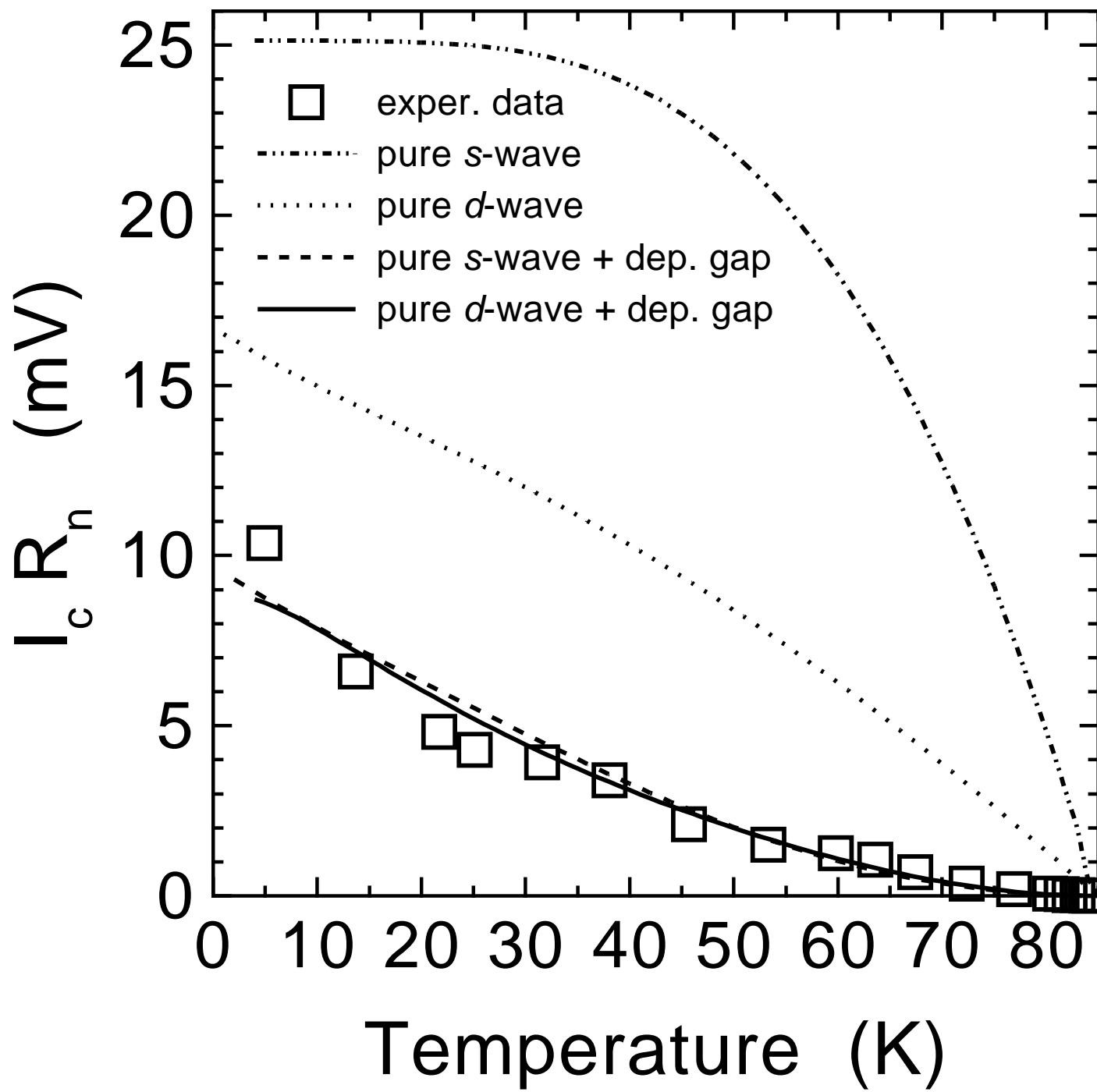
G. A. Ummarino et al., "Intrinsic surface depression of the ...", Fig. 2



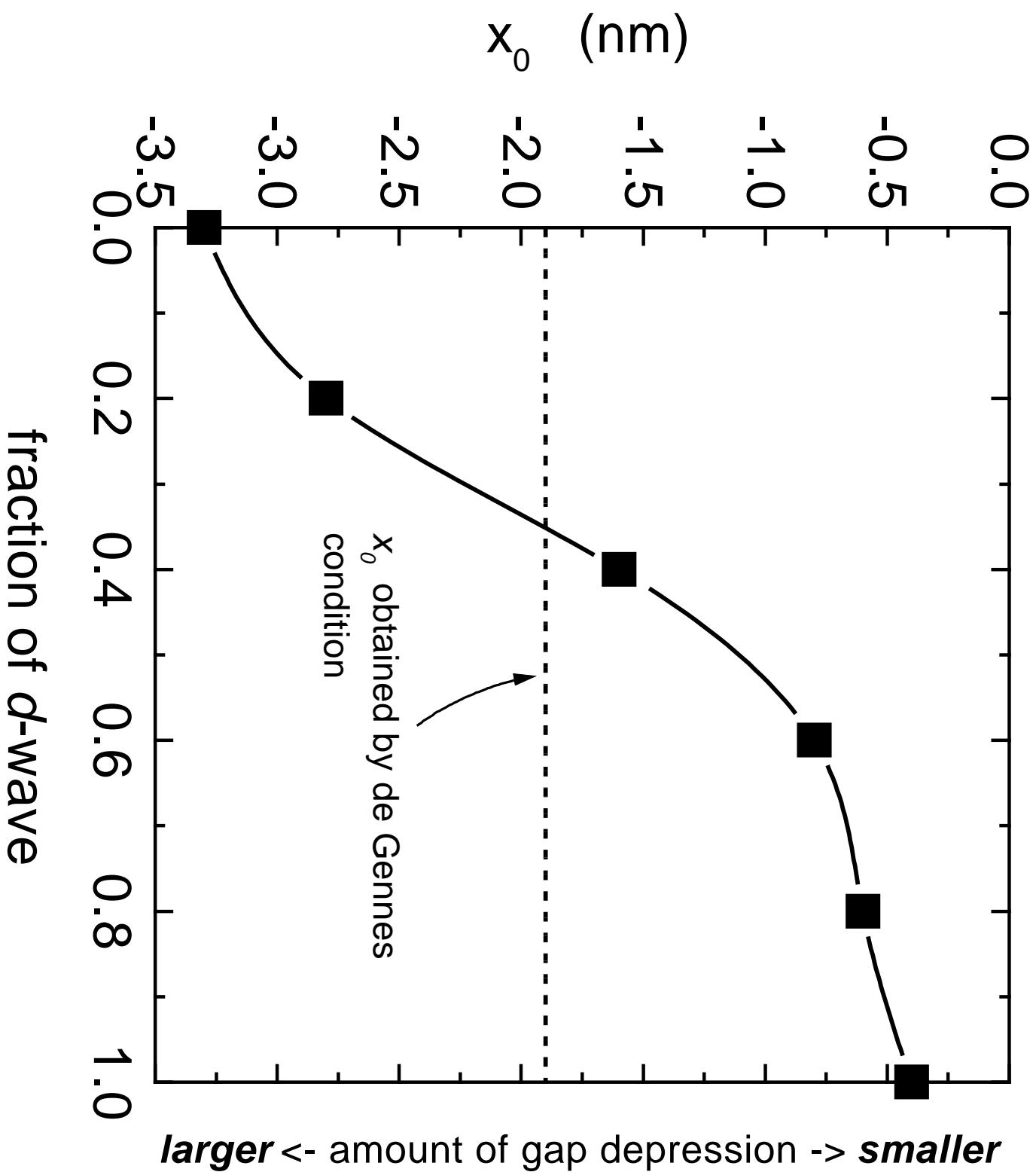
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of the ...", Fig. 3



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of the ...", Fig. 4



G. A. Ummarino et al., "Intrinsic surface depression of the ...", Fig. 5



G. A. Ummarino et al., "Intrinsic surface depression of the ...", Fig. 6